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CHEMICAL DYNAMICS STUDIES OF HIGH ENERGY DENSITY MATERIALS

FINAL TECHNICAL REPORT

(Report Period: August 15, 1992 - August 14, 1996)

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ABSTRACT

The research performed with support by AFOSR (EPSCoR) grant F49620-92-J-0433 (Parent grants: F49620-92-L-0237; F49620-95-1-0310) for the period August 15, 1992 to August 14, 1996 is described. The research objective of this project was to develop theoretical models that can eventually be used for simulations of reactions in solids. The chemical emphasis was on the energetic molecule NTO (5-nitro-2,4-dihydro-3H-1,2,4-triazol-5-one). We carried out a study of the structure and vibrational spectra of the NTO molecule in the gas and solid phases. This work was done in a collaboration with Professor Charles Wight's experimental group (University of Utah). *Ab initio* quauntum mechanical calculations and measured infrared spectra were used to develop potential energy surfaces (valence force fields) for equilibrium NTO in isolation and in a solid phase.

RESEARCH

The research objectives of this research was to develop theoretical models for the simulations of reactions in solids, with particular emphasis on the energetic molecule NTO (5-nitro-2,4-dihydro-3H-1,2,4-triazol-5-one). The purpose of the AFOSR/EPSCoR program under which this grant was made is to provide support for U. S. citizens to do Ph.D. thesis research of interest to DoD.

Studies were carried out, in collaboration with Professor Charles Wight and Mr. David Beardall, University of Utah, of the structure and vibrational spectra of NTO. *Ab initio* molecular orbital theory calculations at the Hartree-Fock and MØller-Plesset levels were performed to determine the structure and vibrational spectra of the NTO. Also, infrared spectra were measured for pure NTO films and NTO isolated in an argon matrix at 21 K. Based on the theoretical results calculated at the MP2/6-311G** level and the measured frequencies, force fields were developed which correspond to isolated molecules and molecules in a solid.

The measured spectra for NTO isolated in an argon matrix and in thin films have significant differences with large and blue shifts of more than 100 cm^{-1}. The largest variations of the peak positions are for the N-H stretches. It is believed that these spectral shifts result from hydrogen bonding in the solid phase. There is relatively good agreement between the scaled *ab initio* frequencies at the MP2/6-311G** level and the values measured for NTO in the Ar matrix. Similar good agreement exists, except for the N-H bond lengths, for the measured geometry of β-NTO and the optimzed geometry at the MP2/6-311G** level.

Density functional theory (DFT) calculations were also carried out. The DFT results demonstrate that the B3LYP exchange-correlation functional gives a good description the NTO molecule. It is similar to that computed at the MP2 level.

The experimental and theoretical results were then used to develop two force field potentials, one for isolated NTO and the other for solid NTO. The results of

normal mode analyses and power spectra at zero-point energies show that these force fields accurately reproduce the *ab initio* and experimental results.

These potential energy surfaces provide the basis for the development of potentials for future studies of NTO in both the gas phase and in solids. Furthermore, this study provides a better understanding of the IR spectral differences in the different phases.

PUBLICATIONS

The following manuscript has been accepted for publication:

Dan C. Sorescu, Teressa R. L. Sutton, Donald L. Thompson, David Beardall, and Charles A. Wight, "Theoretical and Experimental Study of the Structure and Vibrational Spectra of NTO," J. Mol. Spect., in press.

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Mr. Paul Zahner 1.5 years

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